lsopropylpropyzamide 80045-52-9 | DTXSID40230046

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Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 298 °C

Global applicability domain: Inside

Local applicability domain index: 3.51e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

Image not found

Propanil
Measured: 351
Predicted: 317

Image not found

Phenacetin Measured: 244 Predicted: 301 Image not found

3,3-dimethylindolin-2-one

Measured: 300 Predicted: 290

Image not found

Ethyl oxanilate Measured: 280 Predicted: 295 Image not found

N-(2-Methoxyphenyl)acetamide

Measured: 304 Predicted: 301